

10/628,375 2/1/06

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IPC reform
NEWS 8 DEC 23 New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/
USPAT2
NEWS 9 JAN 13 IPC 8 searching in IFIPAT, IFIUIDB, and IFICDB
NEWS 10 JAN 13 New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to
INPADOC
NEWS 11 JAN 17 Pre-1988 INPI data added to MARPAT
NEWS 12 JAN 17 IPC 8 in the WPI family of databases including WPIFV
NEWS 13 JAN 30 Saved answer limit increased
NEWS 14 JAN 31 Monthly current-awareness alert (SDI) frequency
added to TULSA

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FILE 'HOME' ENTERED AT 02:07:04 ON 06 FEB 2006

10/628,375 2/1/06

=> FILE REG

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 02:07:50 ON 06 FEB 2006

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STRUCTURE FILE UPDATES: 3 FEB 2006 HIGHEST RN 873528-70-2

DICTIONARY FILE UPDATES: 3 FEB 2006 HIGHEST RN 873528-70-2

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*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

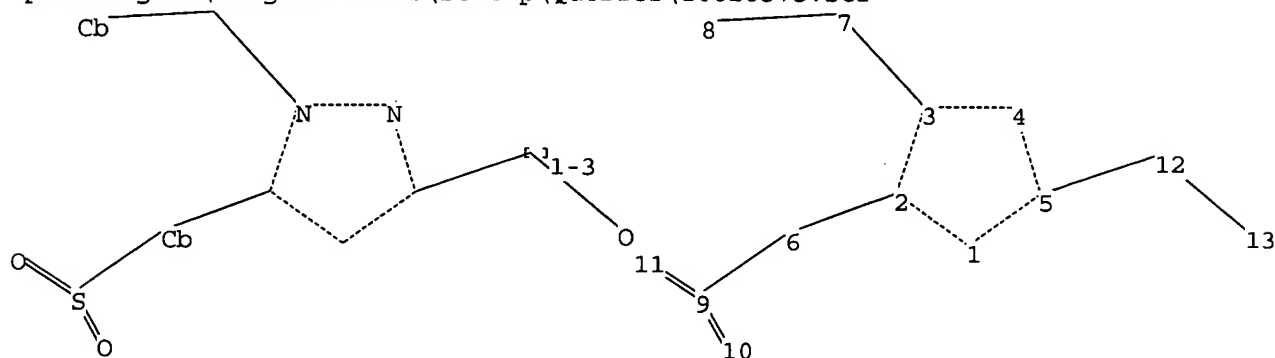
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10628375.str



10/628,375 2/1/06

chain nodes :
6 7 8 9 10 11 12 13
ring nodes :
1 2 3 4 5
chain bonds :
2-6 3-7 5-12 6-9 7-8 9-10 9-11 12-13
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-7 4-5 9-10 9-11 12-13
exact bonds :
2-6 5-12 6-9 7-8
isolated ring systems :
containing 1 :

Match level :

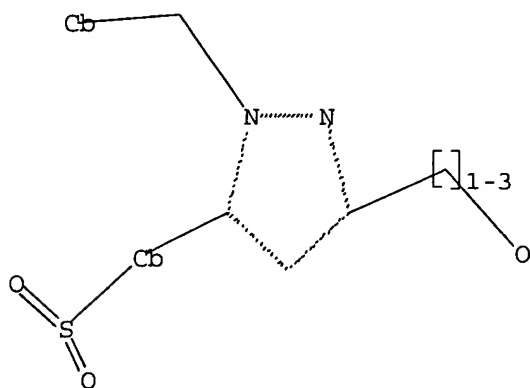
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS

L1 STRUCTURE UPLOADED

=> D

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L1

SAMPLE SEARCH INITIATED 02:08:13 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 541 TO ITERATE

100.0% PROCESSED 541 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 9425 TO 12215

PROJECTED ANSWERS: 0 TO 0

10/628,375 2/1/06

L2 0 SEA SSS SAM L1

=> S L1 FULL

FULL SEARCH INITIATED 02:08:23 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 10476 TO ITERATE

100.0% PROCESSED 10476 ITERATIONS

14 ANSWERS

SEARCH TIME: 00.00.01

L3 14 SEA SSS FUL L1

=> FILE CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'CAPLUS' ENTERED AT 02:08:29 ON 06 FEB 2006

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FILE LAST UPDATED: 5 Feb 2006 (20060205/ED)

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=> S L3

L4 3 L3

=> D IBIB ABS HITSTR TOT

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:252948 CAPLUS

DOCUMENT NUMBER: 140:423618

TITLE: Synthesis and Selective Cyclooxygenase-2 Inhibitory Activity of a Series of Novel, Nitric Oxide Donor-Containing Pyrazoles
 AUTHOR(S): Ranatunge, Ramani R.; Augustyniak, Michael; Bandarage, Upul K.; Earl, Richard A.; Ellis, James L.; Garvey, David S.; Janero, David R.; Letts, L. Gordon; Martino, Allison M.; Murty, Madhavi G.; Richardson, Stewart K.; Schroeder, Joseph D.; Shumway, Matthew J.; Tam, S. Williams; Troche, A. Mark; Young, Delano V.

CORPORATE SOURCE: NitroMed Inc., Bedford, MA, 01730, USA
 SOURCE: Journal of Medicinal Chemistry (2004), 47(9), 2180-2193

CODEN: JMCHAR; ISSN: 0022-2623

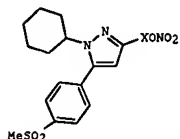
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:423618

GI

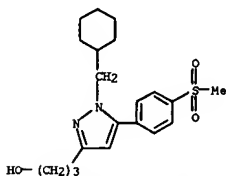


AB The synthesis of a series of novel pyrazoles containing a nitrate (ONO₂) moiety as a nitric oxide (NO)-donor functionality is reported. Their COX-1 and COX-2 inhibitory activities in human whole blood are profiled. The data demonstrate that pyrazole ring substituents play an important role in COX-2 selective inhibition, such that a cycloalkylpyrazole (I, X = CH₂) was found to be a potent and selective COX-2 inhibitor. Other modifications at the 3 position of the central pyrazole ring [I, X = (CH₂)₃, C(:NOH)(CH₂)₃, (2)-CH:CHCH₂CH₂] enhanced COX-2 inhibitory potency. Among the pyrazoles synthesized, the oxime [I, X = C(:NOH)(CH₂)₃] was identified as the most potent COX-2 selective inhibitor. Accordingly, this compound was profiled pharmacol. in the rat after oral administration and shown to possess potent antiinflammatory activity in the carrageenan-induced air-pouch model and less gastric toxicity than a standard

COX-2 inhibitor when administered with background aspirin treatment. The enhanced gastric tolerance of an NO-donor COX-2 selective inhibitor has the potential to augment the clin. profile of this drug class.

IT 654058-48-7P 654058-51-2P 654058-53-4P
 RL: PAC (Pharmacological activity); ACT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant)

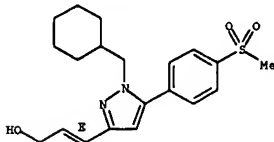
L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



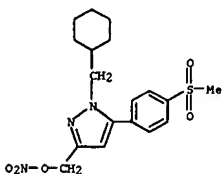
IT 654058-52-3P 654058-60-3P 654058-64-7P
 654058-66-9P 654058-67-0P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and selective cyclooxygenase-2 inhibitory activity of nitric oxide donor-containing pyrazoles)

RN 654058-52-3 CAPLUS
 CN 2-Propen-1-ol, 3-[1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-3-yl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 654058-60-3 CAPLUS
 CN 1H-Pyrazole-3-methanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-, nitrate (ester) (9CI) (CA INDEX NAME)



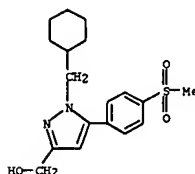
RN 654058-64-7 CAPLUS

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

or reagent)
 (prepn. and selective cyclooxygenase-2 inhibitory activity of nitric oxide donor-contg. pyrazoles)

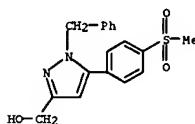
RN 654058-48-7 CAPLUS

CN 1H-Pyrazole-3-methanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RN 654058-51-2 CAPLUS

CN 1H-Pyrazole-3-methanol, 5-[4-(methylsulfonyl)phenyl]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

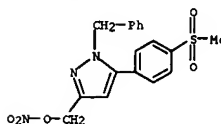


RN 654058-53-4 CAPLUS

CN 1H-Pyrazole-3-propanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

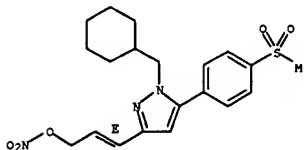
CN 1H-Pyrazole-3-methanol, 5-[4-(methylsulfonyl)phenyl]-1-(phenylmethyl)-, nitrate (ester) (9CI) (CA INDEX NAME)



RN 654058-66-9 CAPLUS

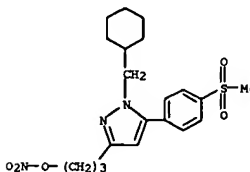
CN 2-Propen-1-ol, 3-[1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-3-yl]-, nitrate (ester), (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 654058-67-0 CAPLUS

CN 1H-Pyrazole-3-propanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-, nitrate (ester) (9CI) (CA INDEX NAME)



REFERENCE COUNT:

52

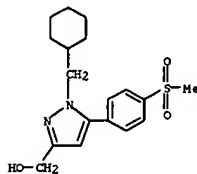
THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2004:100955 CAPLUS
 DOCUMENT NUMBER: 140:157441
 TITLE: Cyclooxygenase-2 selective inhibitors, compositions and methods of use
 INVENTOR(S): Garvey, David S.; Khanapure, Subhash P.; Ranatunge, Raman R.; Richardson, Stewart K.; Schroeder, Joseph D.
 PATENT ASSIGNEE(S): Nitromed, Inc., USA
 SOURCE: PCT Int. Appl., 140 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

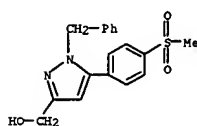
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004010945	A2	20040205	WO 2003-US23605	20030729
WO 2004010945	A3	20040422		
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2493156	AA	20040205	CA 2003-2493156	20030729
US 2004072883	A1	20040415	US 2003-628375	20030729
EP 1542972	A2	20050622	EP 2003-772004	20030729
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005538110	T2	20051215	JP 2004-524981	20030729
PRIORITY APPL. INFO.: US 2002-398829P P 20020729 WO 2003-US23605 W 20030729				

OTHER SOURCE(S): MARPAT 140:157441
 AB The invention describes novel cyclooxygenase 2 (COX-2) selective inhibitors and novel compns. comprising at least one cyclooxygenase 2 (COX-2) selective inhibitor, and, optionally, at least one compound that donates, transfers or releases nitric oxide, stimulates endogenous synthesis of nitric oxide, elevates endogenous levels of endothelium-derived relaxing factor or is a substrate for nitric oxide synthase, and/or at least one therapeutic agent. The invention also provides novel kits comprising at least one COX-2 selective inhibitor, optionally nitrosated and/or nitrosylated, and, optionally, at least one nitric oxide donor, and/or, optionally, at least one therapeutic agent. The novel cyclooxygenase 2 selective inhibitors of the invention can be optionally nitrosated and/or nitrosylated. The invention also provides methods for treating inflammation, pain and fever; for treating and/or improving the gastrointestinal properties of COX-2 selective inhibitors; for facilitating wound healing; for treating and/or preventing renal and/or respiratory toxicity; for treating and/or preventing other disorders resulting from elevated levels of cyclooxygenase-2; and for

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 IT Improving the cardiovascular profile of COX-2 selective inhibitors.
 654058-48-7P 654058-51-2P 654058-52-3P
 654058-53-4P 654058-67-0P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (antiinflammatory cyclooxygenase-2 selective inhibitors)
 RN 654058-48-7 CAPLUS
 CN 1H-Pyrazole-3-methanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



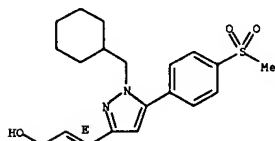
RN 654058-51-2 CAPLUS
 CN 1H-Pyrazole-3-methanol, 5-[4-(methylsulfonyl)phenyl]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



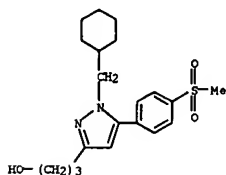
RN 654058-52-3 CAPLUS
 CN 2-Propen-1-ol, 3-[1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-3-yl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

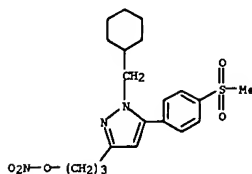
L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 654058-53-4 CAPLUS
 CN 1H-Pyrazole-3-propanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



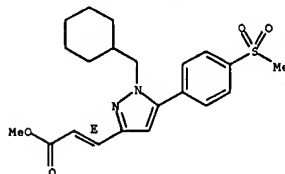
RN 654058-67-0 CAPLUS
 CN 1H-Pyrazole-3-propanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-, nitrate (ester) (9CI) (CA INDEX NAME)



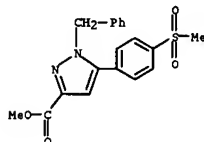
IT 654058-56-7P 654058-58-9P 654058-60-3P
 654058-62-5P 654058-64-7P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (antiinflammatory cyclooxygenase-2 selective inhibitors)
 RN 654058-56-7 CAPLUS
 CN 2-Propenoic acid, 3-[1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-1H-

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 pyrazol-3-yl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

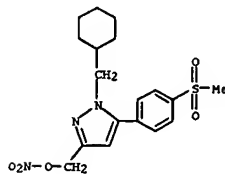
Double bond geometry as shown.



RN 654058-58-9 CAPLUS
 CN 1H-Pyrazole-3-carboxylic acid, 5-[4-(methylsulfonyl)phenyl]-1-(phenylmethyl)-, methyl ester (9CI) (CA INDEX NAME)

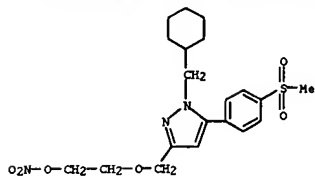


RN 654058-60-3 CAPLUS
 CN 1H-Pyrazole-3-methanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-, nitrate (ester) (9CI) (CA INDEX NAME)

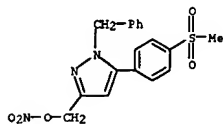


RN 654058-62-5 CAPLUS
 CN Ethanol, 2-[[1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-3-yl]methoxy]-, nitrate (ester) (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS ON STN (Continued)

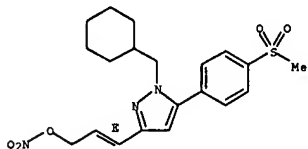


RN 654058-64-7 CAPLUS
 CN 1H-Pyrazole-3-methanol, 5-[4-(methylsulfonyl)phenyl]-1-(phenylmethyl)-, nitrate (ester) (9CI) (CA INDEX NAME)



IT 654058-66-9
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (antiinflammatory cyclooxygenase-2 selective inhibitors)
 RN 654058-66-9 CAPLUS
 CN 2-Propen-1-ol, 3-[1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-3-yl]-, nitrate (ester), (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

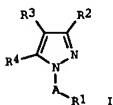


IT 654058-66-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS ON STN

ACCESSION NUMBER: 1999:350656 CAPLUS
 DOCUMENT NUMBER: 131:5254
 TITLE: Preparation of 5-arylpyrazoles as COX-2 selective inhibitors
 INVENTOR(S): Nakamura, Katsuya; Terasaka, Tadashi; Ogino, Takashi; Noda, Yuka; Manabe, Takashi
 PATENT ASSIGNER(S): Fujisawa Pharmaceutical Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 42 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9925695	A1	19990527	WO 1998-JP5041	19981110
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2002509554	T2	20020326	JP 1999-528127	19981110
PRIORITY APPLN. INFO.:			AU 1997-423	A 19971118
			WO 1998-JP5041	W 19981110
OTHER SOURCE(S):		MARPAT 131:5254		
GI				

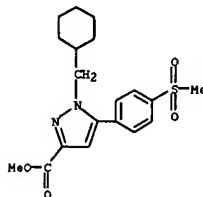


AB The title compds. [I; R1 = (un)substituted aryl; R2 = H, NH2, halo, etc.; R3 = H, aryl optionally substituted with halogen, lower alkyl; R4 = (un)substituted aryl; A = lower alkylene], useful for the treatment and/or prevention of inflammatory conditions, various pains, collagen diseases, autoimmune diseases, various immunity disease, analgesic, thrombosis, cancer or neurodegenerative diseases, were prepared. Thus, refluxing 4,4,4-trifluoro-1-[4-(methylsulfonyl)phenyl]butane-1,3-dione with 3-fluorobenzylhydrazine in AcOH afforded I (A = CH2; R1 = 3-FC6H4; R2 = CF3; R3 = H; R5 = 4-(MeSO2)C6H4) which showed secondary lesion inhibition (uninjected paw) of > 60% at 1.0 mg/kg in rats.

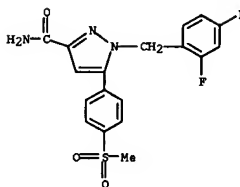
IT 225781-84-0P 225781-90-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of 5-arylpyrazoles as COX-2 selective inhibitors)
 RN 225781-84-0 CAPLUS
 CN 1H-Pyrazole-3-carboxamide, 1-[(2,4-difluorophenyl)methyl]-5-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS ON STN (Continued)

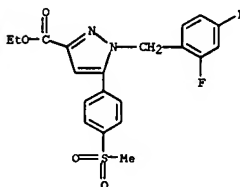
(Reactant or reagent)
 (antiinflammatory cyclooxygenase-2 selective inhibitors)
 RN 654058-86-3 CAPLUS
 CN 1H-Pyrazole-3-carboxylic acid, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS ON STN (Continued)



RN 225781-90-8 CAPLUS
 CN 1H-Pyrazole-3-carboxylic acid, 1-[(2,4-difluorophenyl)methyl]-5-[4-(methylsulfonyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/628,375 2/1/06

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LOGOFF? (Y)/N/HOLD:Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

16.25

183.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-2.25

-2.25

STN INTERNATIONAL LOGOFF AT 02:09:57 ON 06 FEB 2006